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Abstract. A Monte Carlo procedure has been applied in this work in order to address the impact of activation cross sections (XS) uncertainties on contact dose rate and decay heat calculations for the outboard first wall (FW) of a magnetic fusion energy (MFE) demonstration (DEMO) reactor. The XSs inducing the major uncertainty in the prediction of activation related quantities have been identified. Results have shown that for times corresponding to maintenance activities the uncertainties effect is insignificant since the dominant XSs involved in these calculations are based on accurate experimental data evaluations. However, for times corresponding to waste management/recycling activities, the errors induced by the XSs uncertainties, which in this case are evaluated using systematic models, must be considered. It has been found that two particular isotopes, ^{60}Co and ^{94}Nb, are key contributors to the global DEMO FW activation uncertainty results. In these cases, the benefit from further improvements in the accuracy of the critical reaction XSs is discussed.

Keywords: DEMO, activation cross section, uncertainty analysis

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1. INTRODUCTION

Several efforts have previously addressed the effect of activation XS uncertainties in the accuracy of isotopic inventory calculations for Inertial Fusion Energy (IFE) applications [1,2]. In these works, a sensitivity-uncertainty analysis and a Monte Carlo method were proposed to investigate the impact of XS uncertainties on the different radiological inventory response functions. These results showed the suitability of such methods to assess the effect of the uncertainties, and the potential to identify particular reaction XSs that are critical for the overall activation calculation accuracy.

The present work focuses on the application of the Monte Carlo method to predict the impact of XS uncertainties on the decay heat and occupational dose rate in the FW of the MFE DEMO reactor. Isotopes with a dominant contribution to the overall uncertainty of the activation results and their critical reaction XSs are identified here (see Section 3) and recommendations for improving the accuracy of activation calculations regarding the DEMO FW are given.

2. PROBLEM DESCRIPTION AND CALCULATIONAL METHOD

A dual coolant (DC) blanket concept employing a liquid breeder/coolant has been proposed as blanket candidate for a MFE DEMO reactor design [3]. This blanket concept uses high pressure helium to cool the blanket FW and structure, and employs a liquid metal or molten salt (MS) breeder to self-cool the interior of the blanket module, including a beryllium multiplier pebble bed. The structural material for the blanket is the alloy F82H, a low activation ferritic steel (FS). For this work we have used the same F82H elemental composition, including impurities, as that given in reference [4]. In particular, the concentration of Co and Nb impurities is assumed to be 3.4E-03 wt% and 4.00E-4 wt%, respectively. Present reduced activation FS may have higher impurities levels that we have considered in this work. The highest values reported by different laboratories for Co and Nb are 1.00E-02 wt% and 7.00E-04 wt%, respectively [5].

Although there are currently various liquid breeder material options presently under consideration, this work focuses on a blanket design using the low melting point molten salt flibe ($LiBeF_3$). The FW neutron flux intensity is 1.13×10^{15} cm^{-2} s^{-1}, assuming a continuous irradiation of 5 years, which corresponds to the desirable FW lifetime. The average neutron energy is 3.81 MeV. For neutronics and activation calculations, a toroidal cylindrical geometry has been used with the detailed radial build of both the inboard (IB) and outboard (OB) blanket sections [6,7].

The radionuclide inventory, contact γ-dose rate and the decay heat have been calculated using the ACAB [8] code. The nuclear data libraries used for inventory calculation are those from the European Activation File EAF-2003 (EAF_XS, EAF_UN, and EAF_DEC) [9].

The uncertainty analysis has been performed using a Monte Carlo procedure included in the ACAB code, which is based on a simultaneous random sampling of all the XS probability density functions (PDF) involved in a particular problem. The PDF for each XS is assumed to be lognormal [9]. This means that for any XS we can define the random variable $\log(\sigma/\sigma_0)$ that follows a normal distribution $N(0,\Delta)$, with σ_0 being the best-estimate XS value contained in the EAF_XS-2003 XS library, and $\Delta = \Delta_{EAF}/3$, being Δ_{EAF}^2 the variance included in the EAF_UN-2003 library [9]. The uncertainty values included in the EAF_UN-2003 library are defined as three times the experimental standard deviation of σ, that is $\Delta_{EAF} = 3\Delta_{EXPERIMENTAL}$, in order to represent a 99.73% confidence limit.

All results presented in this paper have been obtained with a 1000 histories sample size, which was found appropriate for our applications [2].

3. UNCERTAINTY ANALYSIS FOR DEMO FIRST WALL ACTIVATION

We have obtained the probability distribution for any radiological quantities A, and the corresponding relative error at a 95% confidence level [$E_{95} = (A_{95} - A_0)/A_0$], where A_{95} is the percentile 95 of the probability distribution, and A_0 the nominal value of A from the standard activations calculations, i.e. those using the best estimate XSs. In the present work we have applied the uncertainty analysis previously described to the contact dose rate and the decay heat results at the FW of the DEMO DC concept using the molten salt flibe.

For clarification purposes it should be noted that whenever the term “error” of A is used throughout this work, it refers to the E_{95} value, or relative error at the percentile 95 for the radiological quantity of interest in each case.

3.1 Contact Dose Rate

Figure 1 shows that from the moment of shutdown up to ~4 yrs (1.34×10^8 s), the relative error is less than 6%, therefore the effect of XS uncertainties on the activation results during times relevant for maintenance activities is insignificant. The isotopes that contribute the most to the dose rate and to its associated uncertainty at these times are: ^{56}Mn (from shutdown to ~4.5 hrs), and ^{54}Mn (from a few hours up to 4 yrs) [10].

The starting isotope of the sequences responsible for the main generation of ^{56}Mn and ^{54}Mn is ^{56}Fe, via $^{56}Fe(n,p)^{56}Mn$ and $^{56}Fe(n,2n)^{55}Fe(\beta^+)^{55}Mn(n,2n)^{54}Mn$, respectively. The evaluation of the (n,2n) and (n,p) reactions for ^{56}Fe are well known and the uncertainty associated is small. Therefore, the contact dose relative error is not relevant for FW maintenance activities.

Nevertheless, from a waste management point of view, it is important to assess the calculation error at longer times after shutdown. The uncertainty analysis results show that for times over ~8.5 yrs (2.68×10^8 s) the relative error in the contact dose rate can be as large as 43% (see Figure 1). Such error is mostly due to the uncertainty associated to the inventory prediction of two particular radionuclides: ^{60}Co and ^{94}Nb.

It has been found that at t = 8.5 yrs of cooling, the ^{60}Co contribution to the dose rate is 68% of the total value (36.4 Sv/hr), being the relative error of the dose calculation 29%. The contribution from ^{60}Co reaches a maximum at ~17 yrs after shutdown, being this isotope responsible for almost 100% of the total dose at this time with a relative error of 43%. For longer times, the ^{60}Co contribution starts to decrease, being less than 10% at a time of ~100 yrs, when the error for the total dose has a value of 22%. It is at this time when the ^{94}Nb contribution is the most important, increasing for t >100 yrs. Thus, the relative error of the dose estimation increases again up to ~36% due to ^{94}Nb for longer cooling times.

The generation ^{60}Co is due to the reactions $^{59}Co(n,\gamma)^{60}Co$ and $^{59}Co(n,\gamma\text{-m})\,^{60m}Co$. In the case of ^{94}Nb the critical reactions are $^{93}Nb(n,\gamma)\,^{94}Nb$ and $^{93}Nb(n,\gamma\text{-m})\,^{94m}Nb$. Figure 2 shows the error that each reaction separately induces to the E95. These reactions are responsible of the total E95 at different times after shutdown.

For both ^{59}Co and ^{93}Nb, the radiative capture XS evaluations are based on experimental data. However, in the keV region, uncertainties for the resonance parameters may not be given in the current evaluated data files. In EAF2003/UN, the derivation of these XSs uncertainty in the keV range is based on systematic models due to the lack of experimental information [9]. Also, as most of the neutron capture experiments do not differentiate the ground and isomeric states of the residual nuclei, the uncertainties of each XS may become large and correlated. In EAF2003/UN an uncertainty of the branching ration of $\Delta^2_{BRANCHING}=0.09$ has been adopted when this branching is derived from systematics. Consequently, the XS uncertainties of these reactions in EAF2003/UN remain high and an improved estimation of these reaction XSs would be highly desirable. The XSs identified here have been selected by computing the uncertainty that each reaction separately induces to the global dose, as shown in Table 1.

In particular, those XSs in the energy range (10 eV – 10^5 eV) considered in EAF2003/UN [9] (uncertainties are provided in a three energy group structure) have been found to be the most critical: i) For the reaction ^{59}Co(n,γ-m)^{60m}Co in the energy range of 10-10^5 eV the Δ^2 is 1.0. At 1.07x10^9 s after shutdown, the induced E95 is 30%, being the total E95= 43.1%. ii) For the reaction ^{93}Nb(n,γ-m)^{94m}Nb in the energy range of 10-7.5x10^3 eV the Δ^2 is 1.0. At 3.15x10^{10} s after shutdown, the induced E95 is 29%, being the total E95= 35.7%.

After processing the EAF2003/UN library and collapsing the uncertainty data with our FW neutron spectrum, we found that the total relative error of the radiative capture XSs for ^{59}Co and ^{93}Nb are 30.33% and 23.27%, respectively. To obtain updated uncertainty values of these XSs, covariance files included in the current evaluated data libraries could be processed. In the case of radiative capture of ^{93}Nb, the JENDL3.3 library [11] assigns uncertainties based on experimental data, processing this evaluated library a total relative error of 13.80% is found (no data uncertainties are included in ENDF/B-VI.R8). In the case of ^{59}Co, the data library ENDF/B-VI.R8 [12] assigns uncertainties that are derived from experimental errors and the consideration of systematics, with a total relative error of 9.51% (no data uncertainties in JENDL3.3).

3.2 Decay Heat

The results from the decay heat calculations are consistent with those obtained for the contact dose rate in the previous section. At early times after shutdown, the decay heat value at the reactor FW is critical from the accident analysis point of view. Figure 3 shows that errors are insignificant for times from shutdown up to ~4 yrs of cooling. The dominant isotopes for both the decay heat result and its associated uncertainty at these early times are ^{56}Mn and ^{54}Mn. The same isotopes identified in the previous section.

From the waste management/recycling perspective, the amount of radioactive decay heat is relevant for longer cooling times. We have found that at t = 17 yrs, when the ^{60}Co contribution to the decay heat is 50% of the total, the relative error of the calculation is 22%. This contribution dominates the total decay heat result up to ~100 yrs after shutdown, when the ^{94}Nb contribution starts to increase.

Thus, an improved evaluation of the XSs for the reactions here identified as most critical (^{59}Co(n,γ-m)^{60m}Co and ^{93}Nb(n,γ-m)^{94m}Nb) would also have a significant impact on the DEMO FW decay heat estimations for cooling times > 4yrs.

4. CONCLUSIONS

In this work we have shown that activation XS uncertainties of the impurities present in the alloy F82H induce a significant error in the contact dose rate and decay heat predictions for the first wall of the MFE DEMO DC concept.

An interesting finding is that the error in the contact dose rate and decay heat estimations for early cooling times, which are relevant for maintenance activities and accident analyses, is rather small. The reason for this is that the XSs critical for the generation of the dominant isotopes at early times are well known, and the small associated uncertainty has little impact on the activation results.

However, for longer times (relevant for waste management/recycling options) the relative error in the predicted radiological magnitudes increases significantly. One of the main conclusions of our analysis is that only the inventory predictions for two specific isotopes, ^{60}Co and ^{94}Nb, are responsible for such significant errors at long cooling times. The results presented in this paper show that the improvement of the XSs (n,γ-m) for the isotopes ^{59}Co and ^{93}Nb in the keV energy range would considerably reduce the uncertainty of the contact dose rate and decay heat prediction uncertainty for the DEMO FW.

It is expected that the proper assignment of the uncertainties included in the updated evaluated data XS libraries (i.e., ENDF/B, JENDL) and the inclusion of correlations will improve our uncertainty estimates.

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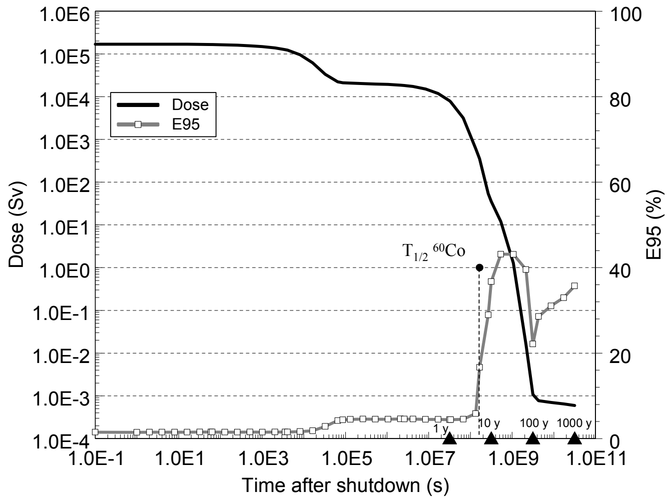

FIGURE 1. Contact dose rate and relative error (E95) for the outboard DEMO blanket FW.

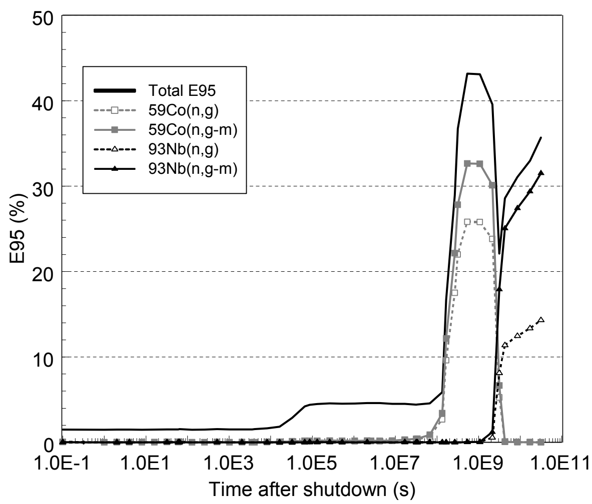

FIGURE 2. E95 total and E95 of major contributors to the total uncertainty of the contact dose rate.

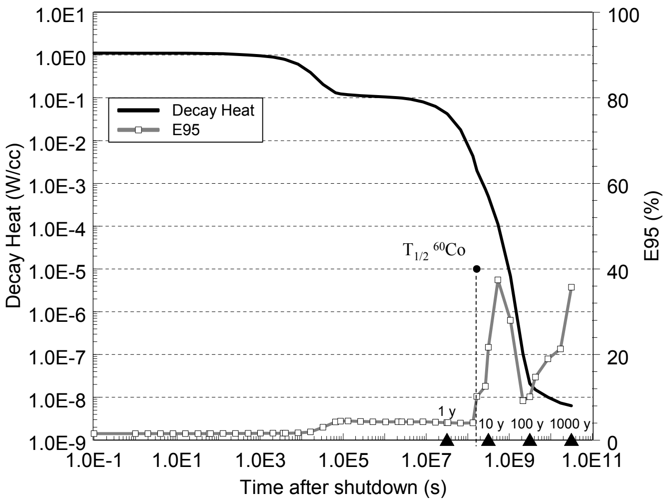

FIGURE 3. Decay heat and relative error (E95) for the outboard DEMO blanket FW.

TABLE 1. E95 for each of the critical reaction cross sections identified in the uncertainty assessment

Time after shutdown (s)	Total E95 (%)	Reaction	Individual effect E95 (%) (Δ^2 uncertainty in EAF2003/UN)		
			Energy Range		
			10^{-5} – 10 eV	10 – 10^5 eV	10^5 – $2x10^7$ eV
$1.07x10^9$	43.1	$^{59}Co(n,\gamma)^{60}Co$	0.2 (Δ^2=0.01)	20.0 (Δ^2=1)	0.2 (Δ^2=0.25)
		$^{59}Co(n,\gamma\text{-}m)^{60m}Co$	0.1 (Δ^2=0.01)	30.0 (Δ^2=1)	1.1 (Δ^2=0.25)
			Energy Range		
			10^{-5} – 10 eV	10 – $7.35x10^3$ eV	$7.5x10^3$ – $2x10^7$ eV
$3.15x10^{10}$	35.7	$^{93}Nb(n,\gamma)^{94}Nb$	1.5 (Δ^2=1)	10.0 (Δ^2=1)	1.0 (Δ^2=0.25)
		$^{93}Nb(n,\gamma\text{-}m)^{94m}Nb$	0.2 (Δ^2=1)	29.0 (Δ^2=1)	6.0 (Δ^2=0.25)